



# HYDROGEN

Energy and Environment Compendium



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# Hydrogen Research at Los Alamos National Laboratory

## The Challenge: Clean Energy and Energy Independence

National and global energy needs are rising as the world population continues to grow and developing countries endeavor to offer their citizens a standard of living that equals that of more developed countries. Recent world events have increased public awareness of the energy, environmental, and security challenges caused by dependence on petroleum imports. To ensure safe, dependable energy supplies for the country and the world, more advanced resources must be developed to meet growing energy needs.

## Hydrogen and Fuel Cells: The Promise and the Challenge

In its 2001 report, the National Energy Policy Development Group declared that hydrogen and other alternative energy technologies show great promise for providing the cleanest possible energy cycle. Hydrogen and fuel cell research have several challenges that must be addressed for innovation to continue in this field:

- **Better understanding of fuel cell system operation**—Conducting basic research to determine how fuel cells and supporting technologies work is the key to enabling knowledge-based innovation.
- **Data acquisition and experimental design**—Understanding and predicting phenomena in operating systems requires advanced diagnostic techniques to gather meaningful data from experiments.
- **Advanced modeling, simulation, and prediction**—Creating integrated models based on fundamental theory and acquired data is essential to understanding fuel cell issues, designing experiments within the model, and predicting fuel cell performance.
- **Proof-of-concept devices and systems**—Evaluating complex devices and systems requires multidisciplinary teams with access to diverse capabilities for innovative proof-of-concept demonstrations.
- **Knowledge and technology transfer**—For benefits in the areas of energy, environmental, and economic security, research and development must lead industry in developing fuel-flexible, efficient, clean, and affordable power systems for widespread use.

## Los Alamos Capabilities in Hydrogen and Fuel Cell Research

In 1977, Los Alamos received Department of Energy funding to begin research into hydrogen as a renewable domestic energy carrier that would reduce emissions-based pollution and lessen the nation's dependence on foreign oil. Los Alamos has been building on this idea ever since.

Hydrogen and fuel cell research at Los Alamos has made significant technological advances in Polymer Electrolyte Membrane (PEM) fuel cells, Direct Methanol Fuel Cells (DMFC), and related technologies including the electrolyzer (a fuel cell in reverse, liberating hydrogen from electricity and pure water). With Los Alamos advances, these technologies may now be used in a variety of civilian power applications, including portable electronics, transportation, and combined heat and power for residential, commercial, and industrial buildings. To address the current scientific challenges faced by the hydrogen and fuel cell research community, Los Alamos has unique expertise and resources in

- **Electrochemical materials and devices**—The Laboratory has the leading expertise in developing fuel cell components (e.g., thin-film electrodes, membrane electrode assemblies, fuel cells, and electrolyzers).
- **Catalyst design, synthesis, characterization, and testing**—Los Alamos has the capability to design, synthesize, characterize, and test both electrocatalysts and catalysts for the various supporting systems.
- **Observational and experimental methods**—With sophisticated observational and experimental methods, the Laboratory can systematically capture fuel cell operation and degradation data.
- **Theory, modeling, and simulation**—Los Alamos has expertise in developing hydrogen- and fuel cell-related models at all scales, from molecular interactions to complete complex power systems.
- **Materials characterization and analytical chemistry**—The Laboratory's expertise in materials characterization and analytical chemistry is key to identifying and resolving fuel cell performance and degradation issues.
- **The Los Alamos knowledge base**—The Laboratory's databases, models, publications, and patent portfolio offer valuable resources to facilitate deeper understanding of phenomena and issues.

- **High-performance computing**—The high-performance computing facilities at the Laboratory provide unparalleled speed that enables researchers to execute complex simulations.
- **Multidisciplinary approaches to complex systems**—Los Alamos approaches scientific and engineering challenges from several directions through expert multidisciplinary teams.

# Hydrogen Fuel Cells for Power and Transportation

## The Challenge: Less Dependence on Petroleum

Energy is consumed largely by three end-use sectors in the United States: buildings, industry, and transportation. Of the three, transportation consumes 27% of total U.S. energy and 67% of U.S. petroleum, and is 95% dependent on petroleum as an energy source. Given recent global events, diversifying the energy sources used to power vehicles has become a widely accepted goal.

## Los Alamos Innovation: Hydrogen-Based Technologies

Recognizing these challenges nearly 30 years ago, Los Alamos began researching and developing means of using hydrogen as a petroleum alternative. In recent years, the Laboratory has developed demonstration hydrogen power systems. In hydrogen-powered transportation, Los Alamos has joined with General Motors (GM) to research methanol fuel processing and cleanup and liquid-fueled electrochemical engines. In the 1990's, Los Alamos and GM collaborated to create the Joint Development Center (JDC). Following the successes of the JDC, the Laboratory continued its own Fuel Cells for Transportation research program for the Department of Energy.

In addition to improving the power density, durability, and efficiency of energy conversion in fuel cells, current Los Alamos efforts are enabling distributed heat and power generation from diverse domestic resources. The project's tasks include

- Exploring ion-transport theory and modeling,
- Performing fundamental electrochemistry,
- Creating innovative devices,
- Researching advanced fuel processing,
- Performing durability studies, and
- Training technicians and researchers in the domestic fuel cell industry.

The program has developed breakthrough thin-film electrode technology which has reduced the amount of platinum required per peak kilowatt by a factor of more than 20 while simultaneously increasing the power density of low-temperature fuel cells. Other program successes include

- Improving fuel cell tolerance to impurities in the fuel stream,
- Improving water management and flow-field/bipolar plate design,
- Developing critical fuel processing components and processes, and
- Optimizing fuel cell design and performance through new understanding and models.

## The Impact: Hydrogen-Based Transportation and Power

These advances have enhanced the viability of fuel cells for transportation. They have also enabled low-temperature fuel cells to be considered for a broad range of consumer applications including cell phones, laptop computers, portable power, and residential and industrial combined heat and power systems. Ultimately, this work at Los Alamos can help enable a transition to a renewable, emission-free hydrogen economy.



Los Alamos National Laboratory researchers were honored for advances in fuel cell technology developed under the collaborative industry-government Partnership for a New Generation of Vehicles.



# Hydrogen Fuel Cells for Common-Use Batteries

## The Challenge: Cheap, Clean, Long-Life Batteries

Conventional batteries used for portable computers, cell phones, flashlights, radios, and wheelchairs are expensive, short-lived, and environmentally unfriendly. Consumers are demanding energy sources that allow longer service without recharging or replacement and that have a longer shelf-life for applications such as flashlights and radios. Fuel cells could provide the long-lived, clean technology ideal for everything from toys to laptops but have traditionally been too complicated and expensive to be practical.

## Los Alamos Innovation: The Air-Breather Fuel Cell Stack

Following its long and successful history of working with U.S. industry to commercialize hydrogen and fuel cell technologies, Los Alamos recently teamed with Enable Fuel Cells Corporation through a cooperative research and development agreement under the DOE Hydrogen Program. Together, Los Alamos and Enable Corp. have developed the breakthrough Air-Breather Fuel Cell Stack technology.

The Air-Breather combines hydrogen and oxygen to produce electricity and water with zero emissions. Unlike its water-hungry predecessors, the Air-Breather (via its membrane electrode assembly) forces water to diffuse out and oxygen to diffuse in. This process requires less humidification and is more water-efficient.

Fuel-cell systems using Air-Breather technology are small, simple, rugged, and inexpensive. They produce only electricity and clean water with no need for additional cooling, reactant compression, or humidification.

Real-world applications of the Air-Breather technology have been tested with good results. These include (1) extending power to the few hundred-watt level, (2) demonstrating a complete power system on a personal mobility vehicle (a 3-wheeled scooter typically used by the elderly or infirm), and (3) commercially licensing to Enable Corp. the technology for battery replacement.

## The Impact: Common Use of Hydrogen Fuel Cells

Hydrogen fuel cells can become the energy source for a host of small-scale applications. Several industries have expressed interest in applying Air-Breather technology to premium products:

- Entertainment/Recreation—cabins, camping, hiking, and sailing.
- Services—search-and-rescue, police, emergency, and military organizations.
- Industry—communications, navigation, telemetry, and computation in remote or inaccessible locations.



**Air-Breather Fuel Cell Stack**

David Garman, right, Department of Energy Assistant Secretary for Energy Efficiency and Renewable Energy, listens as Mahlon Wilson of Electronic and Electrochemical Materials and Devices describes how a hydrogen-powered fuel cell works to power a personal mobility vehicle.



# Hydrogen Storage Innovations to Enable Zero-Emission Vehicles

## The Challenge: Storing Enough Hydrogen Safely

For nearly two decades, the nation's oil use for transportation has grown at an average rate of 2% per year. Consumption for highway vehicles has reached 10 million barrels per day. In addition to dependence on imported energy, oil use for transportation has major environmental effects, producing 79% of U.S. carbon monoxide emissions, 54% of nitrogen oxides emissions, 44% of volatile organic emissions, and 33% of CO<sub>2</sub> (greenhouse gas) emissions. Hydrogen powered vehicles could help solve these problems.

The FreedomCAR Fuel Cell Technology Team and U.S. Department of Energy have identified hydrogen storage as one of the biggest hurdles to introducing zero-emission hydrogen fuel cell vehicles and thus one of the highest priorities in research and development. Current technologies—including storage approaches based on compressed gas, hydrides, and cryogenic liquids—do not, and are not expected to, reach targets incorporating vehicle range, cost, weight, volume, refueling time and ease, and safety.

## Los Alamos Innovation: Chemisorption, Microspheres, and Materials Science

Los Alamos is approaching the hydrogen storage hurdle with a diverse, multidisciplinary group of experts. This team is drawing on Los Alamos's capabilities in materials and surface characterization (including neutron scattering), materials synthesis, and innovative testing and performance characterization methods.

This team's in-depth research and development program for transcending hydrogen storage deficiencies will include investigating (1) chemisorption, (2) polymer microspheres (offering a safe hydrogen storage medium flowing much like a liquid for rapid refueling and storage), and (3) potential storage materials with high-throughput screening and combined approaches.

## The Impact: Zero-Emission Vehicles

Breakthroughs in hydrogen storage at Los Alamos could have impacts beyond the transportation sector with other fuel cell applications including (1) battery replacement and portable power for both civilian and military use and (2) buffer hydrogen storage in renewable-energy and fuel-cell power systems.

Los Alamos efforts are likely to improve the technology to store large quantities of hydrogen in a safe, economical, easily-refillable, energy-efficient, compact, and lightweight configuration—all of which are necessary to make zero emission vehicles a reality. This team's success could elevate hydrogen in the U.S. and the world as a flexible, secure, domestically-produced, and clean energy source.



# Fuel Processing for Fuel Cell Systems

## The Challenge: Developing New Sustainable Power Technologies

Our energy, environmental, and economic security are challenged by current technologies for power production in transportation, buildings, and industry. To achieve the vision of flexible, affordable, safe, domestically-produced energy to be used in all sectors of the economy and in all regions of the country, the nation needs new power technologies that reduce resource depletion and negative environmental impacts.

## Los Alamos Innovation: Integrating Strong Hydrogen Programs into Industry Applications

With nearly 30 years of experience in hydrogen and fuel cells, Los Alamos has been identified by the U.S. Department of Energy as its premier laboratory for hydrogen and fuel cell R&D. Promising developments in power technologies for hydrogen generation at Los Alamos are currently being sponsored by DOE's Office of Energy Efficiency and Renewable Energy and directed by DOE's Office of Hydrogen, Fuel Cells, and Infrastructure Technologies. Los Alamos has also earned an international reputation for scientific and engineering excellence and innovation for two aspects of its work: (1) performing fundamental research to improve the performance and durability of low-temperature fuel cells while simultaneously lowering the cost; and (2) developing fuel processing and associated cleanup technologies to allow hydrogen fuel cells to run off hydrogen-rich gas streams derived from hydrocarbon fuels.

In collaboration with U.S. industry and driven by a commitment to advance multidisciplinary approaches, Los Alamos has achieved the following technology advancements:

- Preferential Oxidation (PrOx) technology and cleanup approaches—transferred to the domestic fuel cell industry for demonstration purposes and now being applied to other fuel-stream trace impurities that cause fuel cell degradation.
- Fundamental modeling and *in situ* characterization techniques—advancing the prospects of even difficult-to-reform fuels such as diesel.
- A significant DOE program to determine the effects of individual fuel components and additives on reforming to help develop a future liquid hydrocarbon fuel for fuel cells.
- An established fuel cell durability program where test cells are operated on real reformat to determine fuel and fuel-processing effects on lifetime and performance.

Features of the pioneering technology at Los Alamos in fuel reformation and cleanup can be found in most, if not all, fuel processing systems for both stationary and transportation fuel cells under development worldwide.

## The Impact: Emission-Free Power for a Secure Energy Future

With strong future programs virtually assured, the technologies advanced by Los Alamos can enable distributed heat and power generation from diverse domestic resources and improve the efficiency of energy conversion. This will enable a transition to a renewable hydrogen economy with emission-free power, and greatly improve national energy, environmental, and economic security.

The cylinder to the left is a preferential oxidation (PrOx) unit connected to a laboratory test apparatus.



# Direct Methanol Fuel Cells for Portable Electronics

## The Challenge: Overcoming Conventional Battery Deficiencies

Many portable electronic devices on the market today require increasing power, but they continue to use conventional batteries that are expensive, short-lived, and environmentally unfriendly. In some applications, such as emergency portable electronics, battery shelf-life can be a problem.

There is significant market pull for batteries that will allow longer service without recharging or replacement. Fuel cells could provide the long-lived, clean technology ideal for portable electronic devices, but in the past they have been too complicated, expensive, and inefficient to be practical. While hydrogen fuel cells offer appropriate power density, with current technology, adequate energy storage is a problem at low power levels.

## Los Alamos Innovation: Direct Methanol Fuel Cells

In an effort to overcome these deficiencies, Los Alamos is developing Direct Methanol Fuel Cell (DMFC) power systems. This project uses the capabilities and expertise developed in more than 20 years of fundamental research and proof-of-concept device development in polymer electrolyte membrane fuel cells at Los Alamos. This work is funded by the U.S. Department of Energy's Office of Energy Efficiency and Renewable Energy through its Office of Hydrogen, Fuel Cells, and Infrastructure Technology.

Los Alamos has performed fundamental research and has developed innovative DMFC power systems that are simpler, smaller, lighter, and more affordable, efficient, and reliable. Laboratory advances have leveraged improvements in materials, structures, operating conditions, and supporting systems and components to largely resolve the performance issues.

Los Alamos has a long and successful history of working with U.S. industry to commercialize fuel cell technologies. Early commercial applications of DMFC technology could include power for cell phones, portable computers, personal digital assistants, and multimedia players. Supported by the DOE, Los Alamos has teamed with Motorola to develop and commercialize DMFC technology at the sub-watt to few-watt levels and licensed its DMFC intellectual property portfolio to MTI Micro Fuel Cells.

## The Impact: Wide Use of Portable Fuel Cells

The innovation and discoveries in methanol fuel cells also support hydrogen fuel cell research and development at the Laboratory to the betterment of both. Future advances are expected to make DMFC's cost-competitive while offering energy density unavailable from batteries. DMFC's may well be one of the first fuel cell systems to penetrate the market and reach volume production. Since they share many materials and features with hydrogen-fueled systems, the commercialization of direct methanol fuel cells will facilitate commercialization of hydrogen systems.



Motorola cell phone powered by a direct methanol fuel cell.

# Direct Methanol Fuel Cells for Portable Power

## The Challenge: New Power Sources for Defense Applications

The U.S. Department of Defense needs lighter and more compact electric power sources for soldiers, robotics, and other emerging applications. The primary and rechargeable batteries currently used for these systems store an insufficient amount of energy to meet the needs of critical future missions.

## Los Alamos Innovation: Breakthroughs in DMFC Technology

The Defense Advanced Research Projects Agency's (DARPA) Palm Power Initiative has funded Los Alamos to develop the science and technology base for a palm power demonstration based on the Laboratory's direct methanol fuel cell work. This project applies capabilities and expertise developed during more than 20 years of fundamental research at Los Alamos, research that has generated many proof-of-concept devices in polymer electrolyte membrane fuel cells.

While past direct methanol fuel cells have had relatively poor performance, Los Alamos has largely solved the problems with technical innovations in membrane materials, catalyst formulation, electrode structures, methanol dilution, and operating temperature. The result is a simple, rugged DMFC that

- Directly oxidizes the high-energy-density hydrogen carrier at the fuel cell anode;
- Allows both high-energy density and rapid refueling and reuse;
- Exceeds the capabilities of traditional fuel cells in size, affordability, and efficiency;
- Adjusts to the desired power characteristics of specific applications; and
- Provides stable and reliable performance with a relatively simple system design.

The high energy density and environmentally benign construction of the DMFC provide distinct advantages over most battery technologies. Further advances are expected to make these systems scalable to higher power levels, like the higher power DMFC portable power systems previously developed by Los Alamos and Ball Aerospace for the Department of Energy in collaboration with the U.S. Army Communications and Electronics Command (CECOM).

## The Impact: Compact, Reliable Portable Power

Early applications of DMFC technology include (1) meeting the portable power needs of the military, intelligence community, police, and other emergency organizations; and (2) serving as dependable, long-lived sources of industrial electricity for communications, navigation, telemetry, and computation in remote or inaccessible locations. Future DMFC power systems may become as ubiquitous as batteries are today.



Two 11-watt fuel cell stacks (above), developed at Los Alamos, are at the core of the DMFC-20 power system (below). The box to the left of the laptop contains fuel for the fuel cells housed in the larger box to the right. This system has up to 10 times the energy density of batteries.



# Future Directions

## Trends and Issues

Concerns with current energy use patterns are rapidly increasing national interest in energy sustainability. Two great concerns are (1) threats from the environmental effects of toxic emissions and greenhouse gases and (2) economic and security vulnerabilities from reliance on imported oil. Alternative energy systems like those based on hydrogen and fuel cells are enjoying both increased press attention and further scientific consideration.

## Goals

Los Alamos is developing a new national initiative to secure and maintain U.S. dominance in hydrogen and fuel cell technology. With the support of the U.S. Department of Energy's Office of Energy Efficiency and Renewable Energy (DOE/EERE), the Laboratory will systematically attack challenges in fuel cell technology. Through collaborations with other national laboratories, universities, and industry, Los Alamos will focus on fuel cell research, application, development, education, training, and enabling technologies in hydrogen production, purification, storage, and safety. These efforts will directly support DOE/EERE goals by enabling a public private partnership that will

- Advance fuel cell technology;
- Develop and validate hardware;
- Train a workforce to meet future fuel cell research and

development demands;

- Accelerate implementation of fuel cell technology to meet domestic needs;
- Significantly advance the timeframe for market introduction of fuel cells; and
- Keep the U.S. ahead of foreign competition.

## Capabilities and Vision

Successful development of innovative technologies is most likely where cornerstone technology and dedicated technical staff already exist. Fuel cell research and development at Los Alamos has the benefit of a world-class reputation and research portfolio as well as its ability to address the key trends facing hydrogen and fuel cell research in the 21<sup>st</sup> century. The Laboratory has unparalleled research power and proven success in

- Electrochemical materials and devices,
- Catalyst design, synthesis, characterization, and testing,
- Observational and experimental methods,
- Theory, modeling, and simulation,
- Multidisciplinary approaches to complex systems,
- Documented knowledge base,
- Polymer electrolyte membrane fuel cell research and development,
- High-performance computing, and
- Collaborations with key U.S. industry leaders.

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